Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:18 PM GMT

PDB ID	:	4XDA
Title	:	Vibrio cholerae O395 Ribokinase complexed with Ribose, ADP and Sodium ion.
Authors	:	Paul, R.; Patra, M.D.; Sen, U.
Deposited on	:	2014-12-19
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

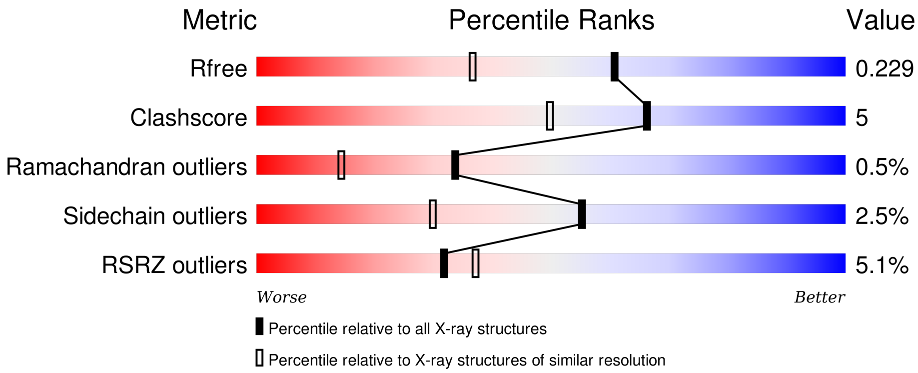
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	309	6% / 88% 11% ••
1	B	309	4% / 87% 12% •
1	C	309	7% / 88% 9% ••
1	D	309	3% / 86% 12% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	RIB	D	401	-	-	-	X
3	ADP	B	402	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10337 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

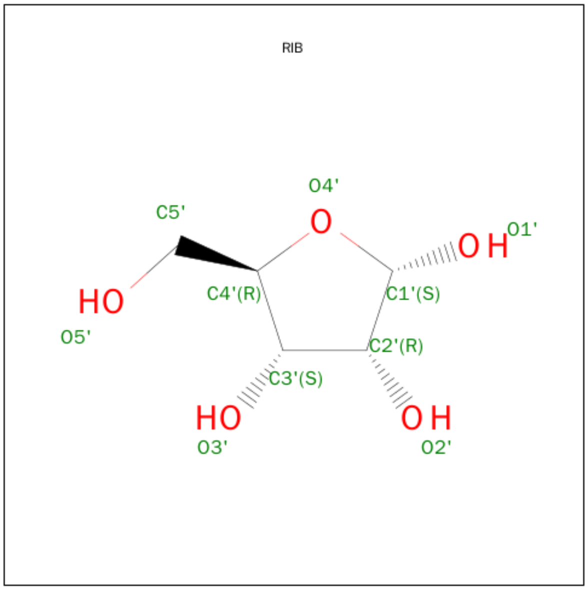
- Molecule 1 is a protein called Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2250	1408	391	441	10	0	0	0
1	B	306	2250	1408	391	441	10	0	0	0
1	C	306	2250	1408	391	441	10	0	0	0
1	D	306	2250	1408	391	441	10	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

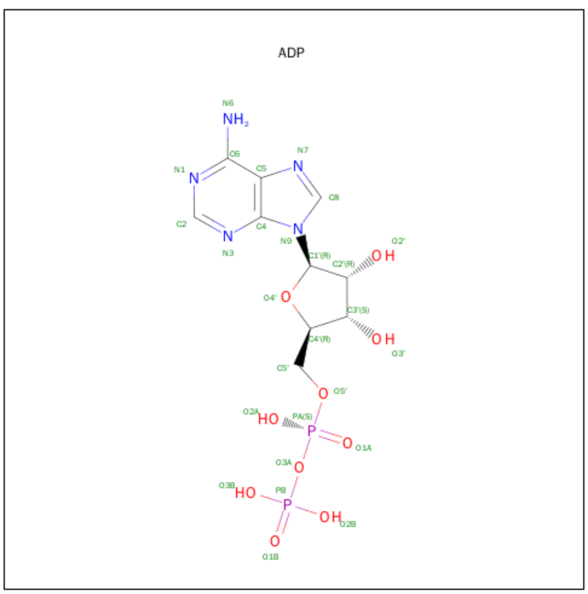
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A5F1B7
A	-1	SER	-	expression tag	UNP A5F1B7
A	0	HIS	-	expression tag	UNP A5F1B7
B	-2	GLY	-	expression tag	UNP A5F1B7
B	-1	SER	-	expression tag	UNP A5F1B7
B	0	HIS	-	expression tag	UNP A5F1B7
C	-2	GLY	-	expression tag	UNP A5F1B7
C	-1	SER	-	expression tag	UNP A5F1B7
C	0	HIS	-	expression tag	UNP A5F1B7
D	-2	GLY	-	expression tag	UNP A5F1B7
D	-1	SER	-	expression tag	UNP A5F1B7
D	0	HIS	-	expression tag	UNP A5F1B7

- Molecule 2 is SUGAR (RIBOSE) (three-letter code: RIB) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 10 5 5	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Na 1	0	0
4	A	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0

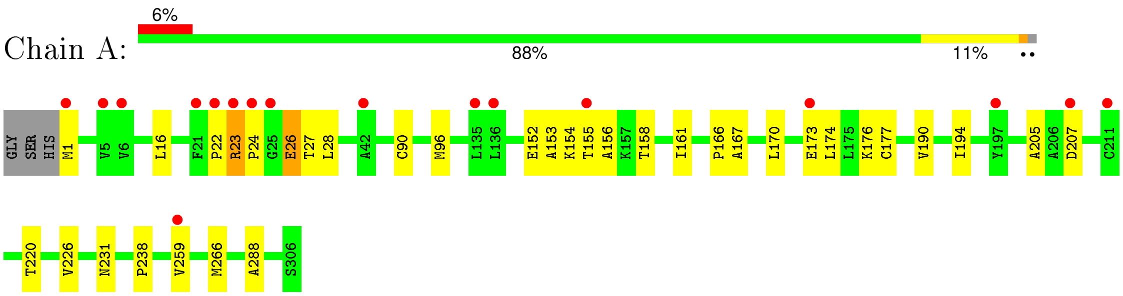
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	281	Total 281	O 281	0	0
5	B	292	Total 292	O 292	0	0
5	C	246	Total 246	O 246	0	0
5	D	349	Total 349	O 349	0	0

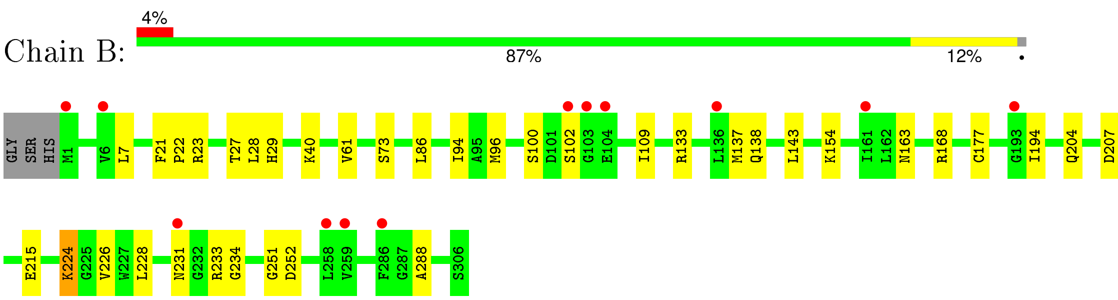
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

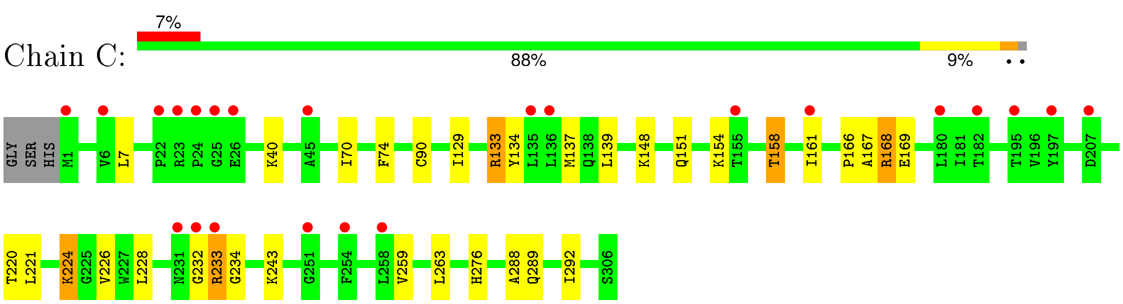
- Molecule 1: Ribokinase



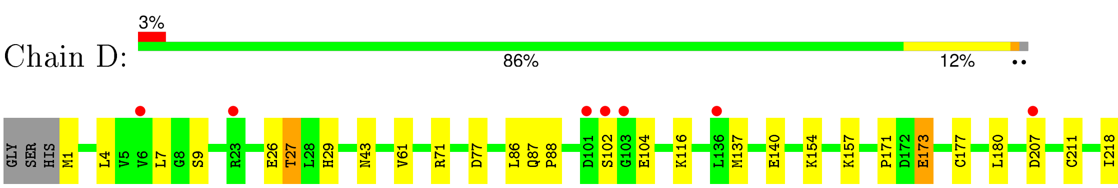
- Molecule 1: Ribokinase

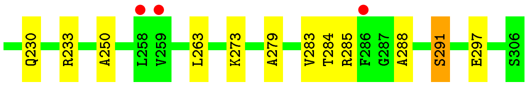


- Molecule 1: Ribokinase



- Molecule 1: Ribokinase




Q230
R233
A250
L258
V259
L263
K273
A279
V283
T284
R285
F286
G287
A288
S291
E297
S306

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.42Å 70.70Å 79.88Å 106.29° 97.65° 98.68°	Depositor
Resolution (Å)	27.42 – 1.75 27.47 – 1.75	Depositor EDS
% Data completeness (in resolution range)	95.9 (27.42-1.75) 85.9 (27.47-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.186 , 0.225 0.195 , 0.229	Depositor DCC
R_{free} test set	5883 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| >$ = 0.47, $< L^2 >$ = 0.30	Xtriage
Outliers	0 of 117298 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10337	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, RIB, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.36	0/2283	0.55	0/3105
1	B	0.38	0/2283	0.54	0/3105
1	C	0.33	0/2283	0.52	0/3105
1	D	0.41	0/2283	0.63	2/3105 (0.1%)
All	All	0.37	0/9132	0.56	2/12420 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	207	ASP	CB-CG-OD1	11.64	128.78	118.30
1	D	207	ASP	CB-CG-OD2	-9.62	109.64	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2250	0	2273	21	0
1	B	2250	0	2273	28	0
1	C	2250	0	2273	21	0
1	D	2250	0	2272	28	0
2	A	10	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10	0	10	0	0
2	D	10	0	10	2	0
3	A	27	0	12	0	0
3	B	54	0	24	6	0
3	C	27	0	12	2	0
3	D	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	281	0	0	3	2
5	B	292	0	0	5	2
5	C	246	0	0	3	1
5	D	349	0	0	9	5
All	All	10337	0	9181	90	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:CYS:SG	5:D:587:HOH:O	2.41	0.78
1:D:288:ALA:O	1:D:291:SER:HB2	1.86	0.75
1:C:220:THR:HA	1:C:226:VAL:HG12	1.76	0.67
1:B:252:ASP:N	3:B:402:ADP:O2B	2.27	0.67
1:C:161:ILE:HD13	1:C:259:VAL:HG22	1.77	0.65
1:D:71:ARG:NH1	5:D:813:HOH:O	2.32	0.62
1:B:40:LYS:HZ2	3:B:402:ADP:PA	2.23	0.60
1:D:273:LYS:NZ	5:D:503:HOH:O	2.32	0.60
1:A:153:ALA:HB1	1:A:158:THR:HB	1.84	0.59
1:C:243:LYS:NZ	5:C:679:HOH:O	2.33	0.58
1:B:73:SER:OG	5:B:792:HOH:O	2.15	0.58
1:A:173:GLU:HA	1:A:176:LYS:HE2	1.84	0.58
1:C:133:ARG:NH2	5:C:732:HOH:O	2.36	0.57
3:C:402:ADP:O3B	5:C:641:HOH:O	2.17	0.57
1:D:157:LYS:NZ	5:D:501:HOH:O	2.30	0.56
1:B:61:VAL:HG23	1:B:86:LEU:HD23	1.86	0.56
1:D:43:ASN:ND2	2:D:401:RIB:H5'1	2.21	0.56
1:B:40:LYS:HG2	3:B:402:ADP:O2A	2.07	0.54
1:A:154:LYS:NZ	1:A:177:CYS:O	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:PRO:HG3	1:D:171:PRO:HB3	1.90	0.53
1:C:129:ILE:O	1:C:158:THR:HG21	2.09	0.53
1:A:194:ILE:HD12	1:A:205:ALA:HA	1.91	0.52
1:A:27:THR:HG21	1:B:109:ILE:HD12	1.91	0.51
1:B:61:VAL:CG2	1:B:86:LEU:HD23	2.41	0.51
1:C:7:LEU:HB3	1:C:137:MET:HG2	1.92	0.51
1:C:40:LYS:HZ1	1:D:27:THR:HG21	1.76	0.51
1:B:233:ARG:NH1	5:B:503:HOH:O	2.44	0.50
1:C:134:TYR:HD1	1:C:161:ILE:HD11	1.76	0.50
1:B:154:LYS:HE3	1:B:177:CYS:O	2.12	0.50
3:B:401:ADP:H8	3:B:401:ADP:O2A	1.95	0.49
1:D:7:LEU:HB3	1:D:137:MET:HG2	1.94	0.49
1:C:167:ALA:N	1:D:26:GLU:OE2	2.43	0.49
1:D:250:ALA:HB2	1:D:283:VAL:HG12	1.94	0.48
1:A:96:MET:HB3	1:B:96:MET:HE3	1.95	0.48
1:B:194:ILE:HD13	1:B:204:GLN:HB3	1.95	0.48
1:A:161:ILE:HD13	1:A:259:VAL:HG22	1.96	0.48
1:D:154:LYS:HE3	1:D:177:CYS:HA	1.95	0.48
1:D:230:GLN:O	1:D:233:ARG:HG2	2.14	0.48
1:D:43:ASN:HD22	2:D:401:RIB:H5'1	1.78	0.47
1:D:9:SER:HB3	1:D:140:GLU:HB3	1.97	0.47
1:A:152:GLU:O	1:A:155:THR:HG22	2.15	0.47
1:C:166:PRO:HG2	1:D:29:HIS:NE2	2.30	0.47
1:C:139:LEU:HD13	1:C:168:ARG:HD2	1.97	0.47
5:A:571:HOH:O	1:D:173:GLU:HG2	2.14	0.47
1:B:251:GLY:N	3:B:402:ADP:O3B	2.44	0.46
1:A:166:PRO:HB3	1:B:27:THR:HB	1.97	0.46
1:C:233:ARG:HB2	1:C:233:ARG:HH11	1.80	0.46
1:A:16:LEU:HD21	1:B:94:ILE:HD11	1.98	0.46
1:B:154:LYS:HG3	1:B:177:CYS:SG	2.56	0.46
1:B:7:LEU:HB3	1:B:137:MET:HG2	1.98	0.45
1:C:224:LYS:N	1:C:224:LYS:HD2	2.32	0.45
1:A:23:ARG:NH1	1:A:26:GLU:OE1	2.49	0.45
1:A:170:LEU:HD22	1:A:174:LEU:HD23	1.99	0.45
1:B:215:GLU:HG3	1:B:231:ASN:ND2	2.31	0.45
1:D:180:LEU:HD21	1:D:218:ILE:HD12	1.99	0.45
1:D:279:ALA:O	1:D:283:VAL:HG13	2.16	0.44
1:B:40:LYS:NZ	3:B:402:ADP:PA	2.90	0.44
1:C:134:TYR:CD1	1:C:161:ILE:HD11	2.52	0.44
1:B:133:ARG:NH2	5:B:504:HOH:O	2.45	0.44
1:A:24:PRO:HA	1:B:21:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ARG:HH22	1:D:297:GLU:CD	2.21	0.44
1:D:61:VAL:HG23	1:D:86:LEU:HD12	2.00	0.43
1:D:233:ARG:NH1	5:D:849:HOH:O	2.51	0.43
1:B:21:PHE:HA	1:B:22:PRO:HD3	1.84	0.43
1:D:87:GLN:HA	1:D:88:PRO:HD3	1.88	0.43
1:A:167:ALA:HB1	1:A:190:VAL:HG21	2.00	0.43
1:A:166:PRO:HG2	1:B:29:HIS:NE2	2.33	0.43
1:C:289:GLN:HA	1:C:292:ILE:HD12	2.00	0.43
1:D:4:LEU:HB2	1:D:263:LEU:HD11	1.99	0.43
1:A:156:ALA:O	5:A:566:HOH:O	2.21	0.43
1:C:148:LYS:HA	1:C:151:GLN:HE21	1.84	0.43
1:C:168:ARG:NH1	1:C:169:GLU:O	2.45	0.42
1:B:143:LEU:HD22	1:B:168:ARG:NH2	2.34	0.42
1:D:27:THR:HG23	5:D:828:HOH:O	2.19	0.42
1:A:220:THR:HA	1:A:226:VAL:HG12	2.02	0.42
1:C:276:HIS:ND1	3:C:402:ADP:O2’	2.49	0.42
1:B:215:GLU:HG3	1:B:231:ASN:HD21	1.84	0.42
1:B:138:GLN:HA	1:B:163:ASN:O	2.20	0.42
1:A:22:PRO:HD3	1:A:28:LEU:HD22	2.02	0.42
1:D:116:LYS:NZ	5:D:505:HOH:O	2.49	0.42
1:C:228:LEU:O	1:C:234:GLY:HA2	2.20	0.41
1:B:102:SER:OG	5:B:698:HOH:O	2.22	0.41
1:C:70:ILE:HG13	1:C:74:PHE:CZ	2.55	0.41
1:D:77:ASP:OD2	5:D:785:HOH:O	2.22	0.41
1:A:266:MET:O	5:A:724:HOH:O	2.22	0.41
1:B:224:LYS:HG2	5:B:790:HOH:O	2.20	0.41
1:A:154:LYS:HA	1:A:154:LYS:HD3	1.95	0.40
1:B:228:LEU:O	1:B:234:GLY:HA2	2.21	0.40
1:C:221:LEU:O	1:C:224:LYS:HB2	2.21	0.40
1:D:1:MET:HA	5:D:837:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:541:HOH:O	5:D:793:HOH:O[1_556]	2.08	0.12
5:A:541:HOH:O	5:D:568:HOH:O[1_556]	2.14	0.06
5:B:551:HOH:O	5:D:516:HOH:O[1_456]	2.15	0.05
5:B:542:HOH:O	5:D:544:HOH:O[1_556]	2.16	0.04
5:C:741:HOH:O	5:D:590:HOH:O[1_545]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/309 (98%)	295 (97%)	7 (2%)	2 (1%)	26	10
1	B	304/309 (98%)	297 (98%)	6 (2%)	1 (0%)	46	25
1	C	304/309 (98%)	296 (97%)	6 (2%)	2 (1%)	26	10
1	D	304/309 (98%)	300 (99%)	3 (1%)	1 (0%)	46	25
All	All	1216/1236 (98%)	1188 (98%)	22 (2%)	6 (0%)	34	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	288	ALA
1	D	102	SER
1	A	288	ALA
1	C	288	ALA
1	A	231	ASN
1	C	232	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/239 (99%)	232 (98%)	5 (2%)	61	37
1	B	237/239 (99%)	231 (98%)	6 (2%)	55	30
1	C	237/239 (99%)	229 (97%)	8 (3%)	44	18
1	D	237/239 (99%)	232 (98%)	5 (2%)	61	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	948/956 (99%)	924 (98%)	24 (2%)	55	30

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	ARG
1	A	26	GLU
1	A	90	CYS
1	A	207	ASP
1	B	23	ARG
1	B	28	LEU
1	B	100	SER
1	B	207	ASP
1	B	224	LYS
1	B	226	VAL
1	C	90	CYS
1	C	133	ARG
1	C	154	LYS
1	C	158	THR
1	C	168	ARG
1	C	224	LYS
1	C	233	ARG
1	C	263	LEU
1	D	27	THR
1	D	104	GLU
1	D	173	GLU
1	D	284	THR
1	D	291	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	B	230	GLN
1	C	98	GLN
1	D	98	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RIB	A	401	-	10,10,10	1.05	1 (10%)	12,14,14	1.38	1 (8%)
3	ADP	A	402	-	22,29,29	0.94	1 (4%)	27,45,45	1.67	3 (11%)
3	ADP	B	401	-	22,29,29	1.08	1 (4%)	27,45,45	1.87	3 (11%)
3	ADP	B	402	-	22,29,29	1.15	1 (4%)	27,45,45	2.79	11 (40%)
2	RIB	C	401	-	10,10,10	0.91	1 (10%)	12,14,14	1.07	1 (8%)
3	ADP	C	402	-	22,29,29	1.08	1 (4%)	27,45,45	1.81	4 (14%)
2	RIB	D	401	-	10,10,10	1.15	1 (10%)	12,14,14	1.54	3 (25%)
3	ADP	D	402	-	22,29,29	1.06	2 (9%)	27,45,45	1.92	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RIB	A	401	-	-	0/2/18/18	0/1/1/1
3	ADP	A	402	-	-	0/12/32/32	0/3/3/3
3	ADP	B	401	-	-	0/12/32/32	0/3/3/3
3	ADP	B	402	-	-	0/12/32/32	0/3/3/3
2	RIB	C	401	-	-	0/2/18/18	0/1/1/1
3	ADP	C	402	-	-	0/12/32/32	0/3/3/3
2	RIB	D	401	-	-	0/2/18/18	0/1/1/1
3	ADP	D	402	-	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	RIB	C1'-C2'	-2.77	1.49	1.52
2	A	401	RIB	O4'-C4'	-2.75	1.38	1.45
2	C	401	RIB	O4'-C4'	-2.23	1.39	1.45
3	D	402	ADP	C2-N3	2.01	1.35	1.32
3	A	402	ADP	C5-C4	2.95	1.47	1.40
3	D	402	ADP	C5-C4	2.99	1.47	1.40
3	B	402	ADP	C5-C4	3.13	1.47	1.40
3	B	401	ADP	C5-C4	3.20	1.47	1.40
3	C	402	ADP	C5-C4	3.31	1.48	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	ADP	N3-C2-N1	-8.12	122.68	128.89
3	D	402	ADP	N3-C2-N1	-7.96	122.80	128.89
3	B	401	ADP	N3-C2-N1	-7.61	123.07	128.89
3	C	402	ADP	N3-C2-N1	-7.02	123.52	128.89
3	A	402	ADP	N3-C2-N1	-5.74	124.50	128.89
3	B	402	ADP	C5'-C4'-C3'	-4.97	95.47	115.21
3	B	402	ADP	O4'-C1'-N9	-4.92	97.80	108.10
3	B	402	ADP	O5'-C5'-C4'	-4.12	93.92	109.12
3	A	402	ADP	PA-O3A-PB	-3.69	120.30	132.67
3	D	402	ADP	PA-O3A-PB	-3.50	120.94	132.67
2	A	401	RIB	O1'-C1'-O4'	-3.48	106.65	111.22
3	B	402	ADP	O3A-PA-O5'	-3.48	93.72	102.94
3	B	402	ADP	C4-C5-N7	-3.07	106.66	109.48
3	C	402	ADP	PA-O3A-PB	-3.01	122.56	132.67
3	A	402	ADP	C4-C5-N7	-2.97	106.75	109.48
2	C	401	RIB	O1'-C1'-O4'	-2.84	107.50	111.22
3	B	402	ADP	PA-O3A-PB	-2.77	123.39	132.67
3	C	402	ADP	C4-C5-N7	-2.75	106.95	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	RIB	O1'-C1'-O4'	-2.52	107.91	111.22
3	C	402	ADP	C2'-C1'-N9	-2.47	110.53	114.29
3	B	401	ADP	C4-C5-N7	-2.29	107.37	109.48
3	B	401	ADP	C2-N1-C6	2.15	122.60	118.77
3	B	402	ADP	C2-N1-C6	2.16	122.63	118.77
2	D	401	RIB	O3'-C3'-C4'	2.35	118.11	111.05
3	B	402	ADP	O3'-C3'-C2'	2.38	119.56	111.83
3	B	402	ADP	O3B-PB-O2B	2.70	117.67	107.38
2	D	401	RIB	C1'-C2'-C3'	3.22	106.72	102.45
3	B	402	ADP	O4'-C4'-C3'	3.33	111.86	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	ADP	1	0
3	B	402	ADP	5	0
3	C	402	ADP	2	0
2	D	401	RIB	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	306/309 (99%)	0.14	17 (5%)	28	33	14, 25, 49, 69	0
1	B	306/309 (99%)	0.15	12 (3%)	43	48	13, 23, 43, 68	1 (0%)
1	C	306/309 (99%)	0.45	23 (7%)	17	22	17, 32, 52, 76	0
1	D	306/309 (99%)	0.12	10 (3%)	50	56	14, 22, 41, 67	0
All	All	1224/1236 (99%)	0.22	62 (5%)	32	37	13, 25, 48, 76	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	GLY	8.9
1	D	286	PHE	4.9
1	A	155	THR	4.5
1	B	103	GLY	4.0
1	B	102	SER	3.8
1	C	25	GLY	3.7
1	C	1	MET	3.6
1	C	23	ARG	3.5
1	B	1	MET	3.4
1	A	1	MET	3.3
1	C	136	LEU	3.2
1	A	136	LEU	3.2
1	C	207	ASP	3.1
1	D	101	ASP	3.0
1	A	207	ASP	2.9
1	A	211	CYS	2.9
1	C	135	LEU	2.9
1	C	197	TYR	2.9
1	B	259	VAL	2.8
1	D	207	ASP	2.7
1	B	231	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	182	THR	2.7
1	C	22	PRO	2.7
1	A	25	GLY	2.6
1	C	6	VAL	2.6
1	A	23	ARG	2.6
1	C	233	ARG	2.6
1	C	231	ASN	2.6
1	C	45	ALA	2.6
1	C	161	ILE	2.6
1	D	102	SER	2.5
1	D	23	ARG	2.5
1	A	24	PRO	2.5
1	C	24	PRO	2.5
1	D	258	LEU	2.5
1	A	6	VAL	2.4
1	B	136	LEU	2.4
1	D	6	VAL	2.4
1	A	259	VAL	2.4
1	D	136	LEU	2.4
1	A	135	LEU	2.3
1	A	173	GLU	2.3
1	C	251	GLY	2.3
1	C	258	LEU	2.3
1	B	258	LEU	2.2
1	B	104	GLU	2.2
1	C	232	GLY	2.2
1	C	195	THR	2.2
1	A	21	PHE	2.1
1	C	26	GLU	2.1
1	C	155	THR	2.1
1	A	22	PRO	2.1
1	A	5	VAL	2.1
1	B	6	VAL	2.1
1	D	259	VAL	2.1
1	B	161	ILE	2.1
1	A	197	TYR	2.0
1	B	193	GLY	2.0
1	C	180	LEU	2.0
1	A	42	ALA	2.0
1	B	286	PHE	2.0
1	C	254	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	RIB	D	401	10/10	0.85	0.17	4.95	30,38,55,64	0
3	ADP	B	402	27/27	0.89	0.19	4.49	13,30,136,200	0
3	ADP	B	401	27/27	0.90	0.12	1.40	16,22,62,105	0
3	ADP	C	402	27/27	0.86	0.15	1.36	29,38,127,151	0
4	NA	B	403	1/1	0.97	0.13	1.22	30,30,30,30	0
3	ADP	D	402	27/27	0.86	0.13	1.20	16,20,70,177	0
3	ADP	A	402	27/27	0.95	0.11	0.88	18,28,146,159	0
4	NA	D	403	1/1	0.94	0.14	0.27	27,27,27,27	0
4	NA	C	403	1/1	0.94	0.07	-0.35	26,26,26,26	0
2	RIB	C	401	10/10	0.95	0.10	-0.40	18,22,31,36	0
2	RIB	A	401	10/10	0.95	0.10	-0.47	15,19,25,31	0
4	NA	A	403	1/1	0.97	0.05	-1.56	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.